



Equilibrium sampling for a thermodynamic assessment of contaminated sediments

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Equilibrium sampling for a thermodynamic assessment of contaminated sediments

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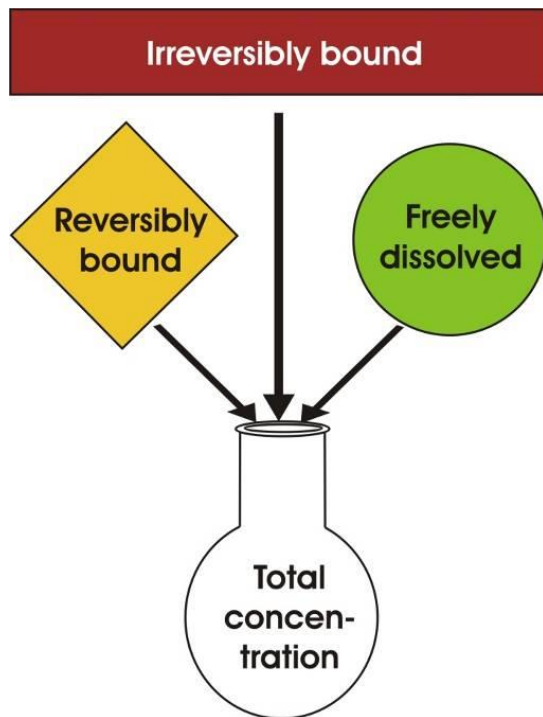
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Equilibrium sampling for a thermodynamic assessment of contaminated sediments

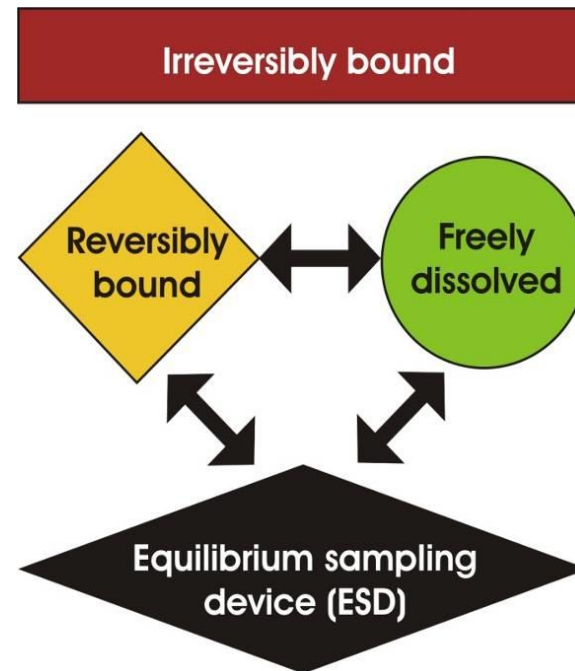
Philipp Mayer¹, Stine N. Schmidt¹, Kimmo Mäenpää²,
Gesine Witt³, Sabine Schäfer⁴, Phil Gidley⁵ & Annika Jahnke⁶

¹Technical University of Denmark, ²University of Eastern Finland, ³Hamburg University of Applied Sciences, Germany, ⁴German Federal Institute of Hydrology, ⁵USACE-ERDC, USA & ⁶Stockholm University, Sweden (now UFZ, Germany)

Classical extraction



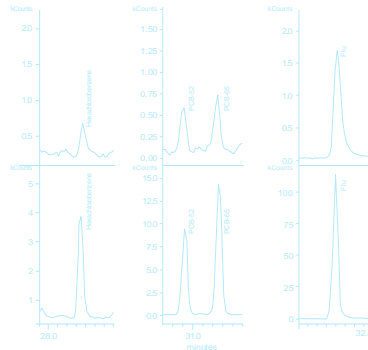
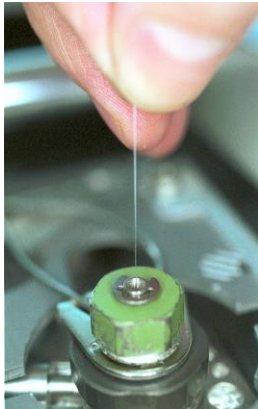
Equilibrium sampling device (ESD)



1) Matrix-SPME with disposable fibers (2000)



1. Equilibrate thin polymer with sample



2. Measure C_{PDMS}

$$3. C_{free} = C_{PDMS} / K_{PDMS,water}$$

Mayer et al, ES&T, 2000, V 34: 5177-5183

Mayer et al., ES&T, 2003, V37: 184A-191A

2) Silicone coated vials (2008)

Chemistry Central Journal

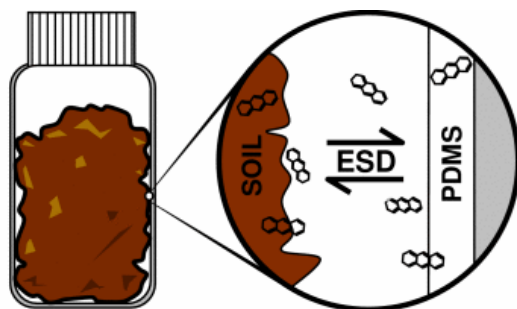
Methodology

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Determining the chemical activity of hydrophobic organic compounds in soil using polymer coated vials

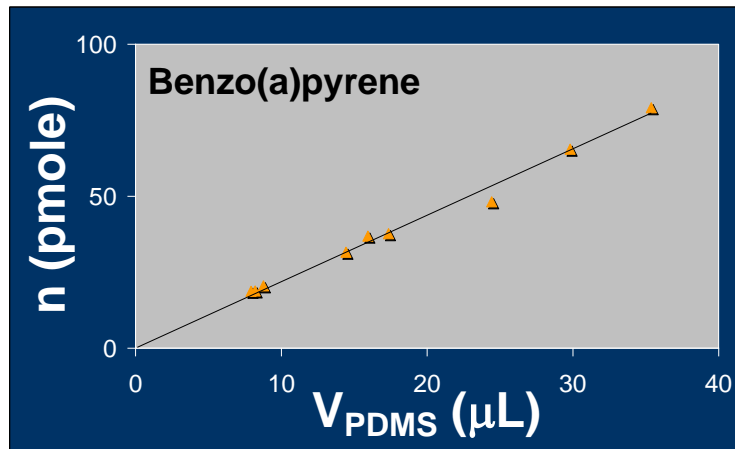
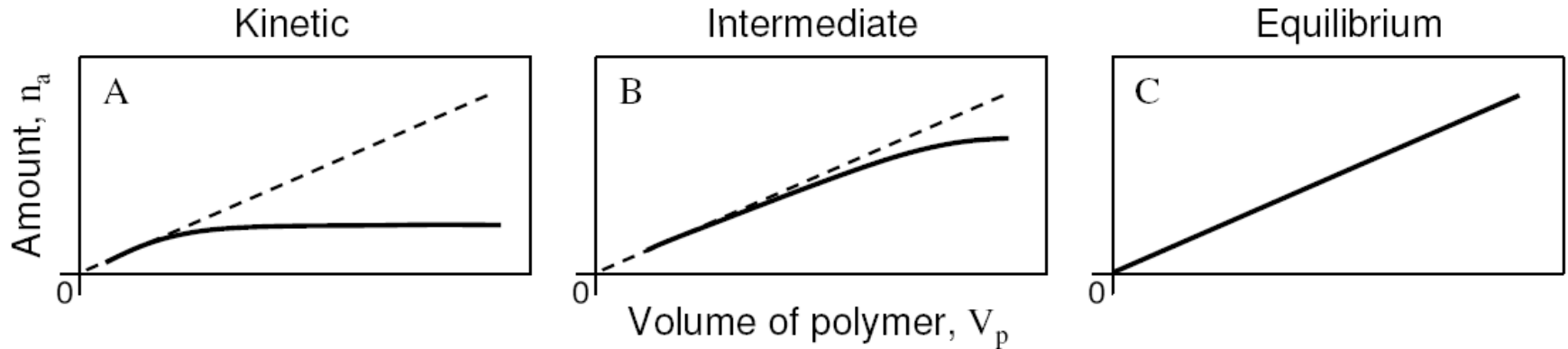
Fredrik Reichenberg^{1,2}, Foppe Smedes³, Jan-Åke Jönsson² and Philipp Mayer*¹

Address: ¹Department of Environmental Chemistry and Microbiology, National Environmental Research Institute, University of Aarhus, PO Box 358, 4000 Roskilde, Denmark, ²Division of Analytical Chemistry, Lund University, PO Box 124, S-221 00 Lund, Sweden and ³Ministry of Transport, Public Works and Water management, National Institute for Coastal and Marine Management/RIKZ, PO Box 207, 9750 AE Haren, Netherlands



Drawing of equilibrium sampling device (ESD) for determination of thermodynamic activity by partitioning to micrometer thin polydimethylsiloxane (PDMS).

Coated vials with multiple coating thickness



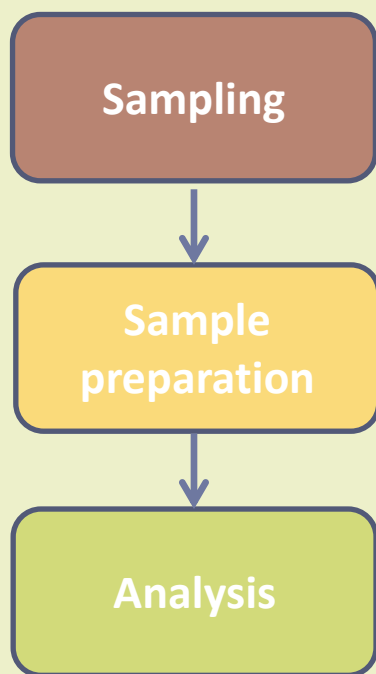
Confirms:

1. equilibrium
2. negligible depletion
3. no surface artefacts/abrasion

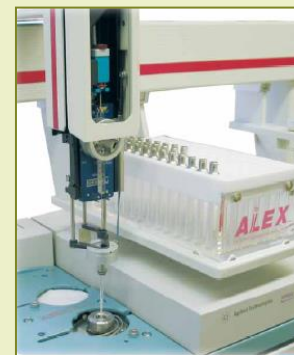
3)

Passive Equilibrium Sampler for in Situ Measurements of Freely Dissolved Concentrations of Hydrophobic Organic Chemicals in Sediments

Gesine Witt,^{*,†} Susann-Cathrin Lang,[†] Dagny Ullmann,[†] Gotja Schaffrath,[†] Detlef Schulz-Bull,[‡] and Philipp Mayer[§]



- **in-situ deployment of sampler**
- **rinse with water and wipe dry**
- **store fiber in GC injection liner**
- **insert fiber with automated injection liner exchange (ALEX)**
- **thermal desorption**
- **MS identification/ quantification**



Measurement endpoints of Equilibrium Sampling

PCB concentrations in polymer $C_{\text{polymer} \rightleftharpoons \text{sed}}$ can be converted into:

1) The effective concentration driving diffusion

$$C_{\text{free}} (g L^{-1}) = \frac{C_{\text{polymer} \rightleftharpoons \text{sed}} (g kg^{-1})}{K_{\text{polymer}:\text{water}} (L kg^{-1})} \quad (\text{since 2000})$$

2) The chemical activity (energetic state) driving equilibrium partitioning

$$a (\text{unit less}) \cong \frac{C_{\text{free}} (g L^{-1})}{S_L (g L^{-1})} \quad (\text{since 2006})$$

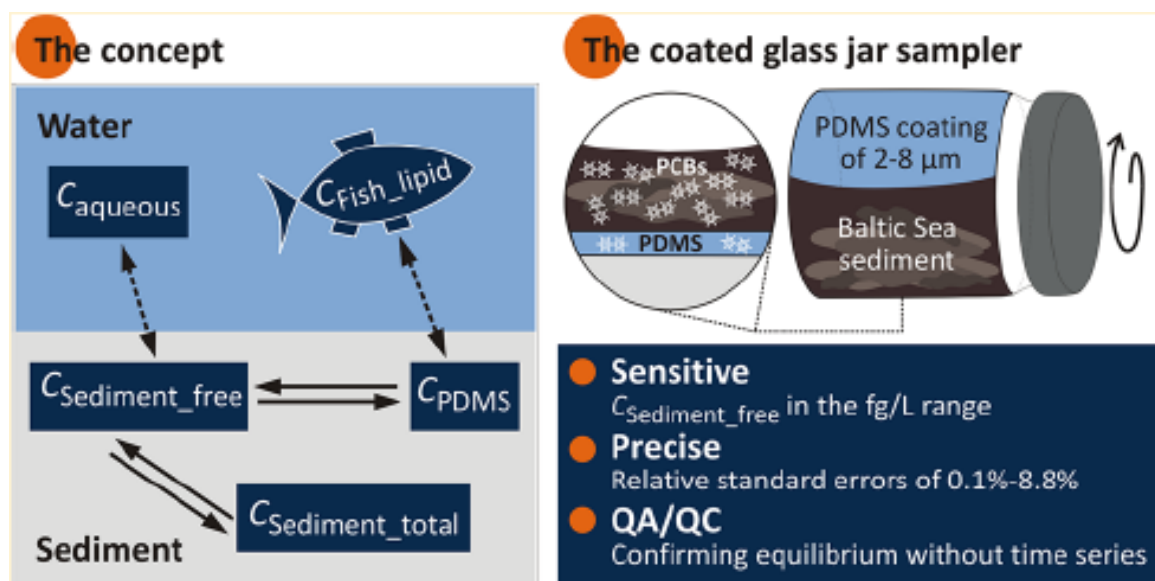
3) The thermodynamic potential for bioaccumulation

$$C_{\text{lip} \rightleftharpoons \text{sed}} (g kg^{-1}) = C_{\text{polymer} \rightleftharpoons \text{sed}} (g kg^{-1}) \times K_{\text{lip:pol}} (kg kg^{-1}) \quad (\text{since 2011})$$

Case Studies focusing on PCBs & $\mathcal{C}_{lip \rightleftharpoons sed}$

Sensitive Equilibrium Sampling To Study Polychlorinated Biphenyl Disposition in Baltic Sea Sediment

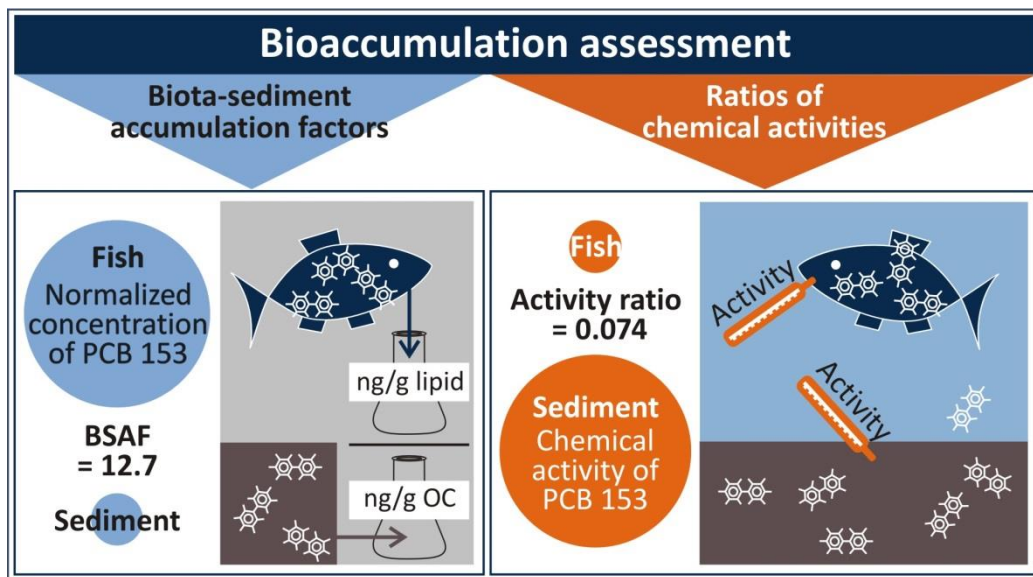
Annika Jahnke,^{*,†} Philipp Mayer,[‡] and Michael S. McLachlan[†]



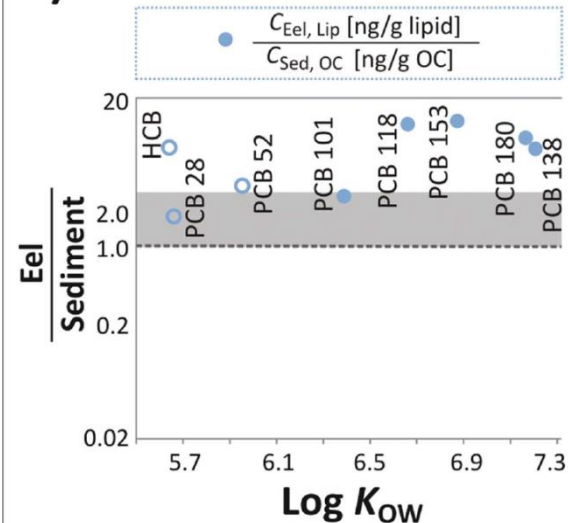
Silicone passive equilibrium samplers as 'chemometers' in eels and sediments of a Swedish lake†

Annika Jahnke,^{*a} Philipp Mayer,^{bc} Michael S. McLachlan,^a Håkan Wickström,^d Dorothea Gilbert^c and Matthew MacLeod^a

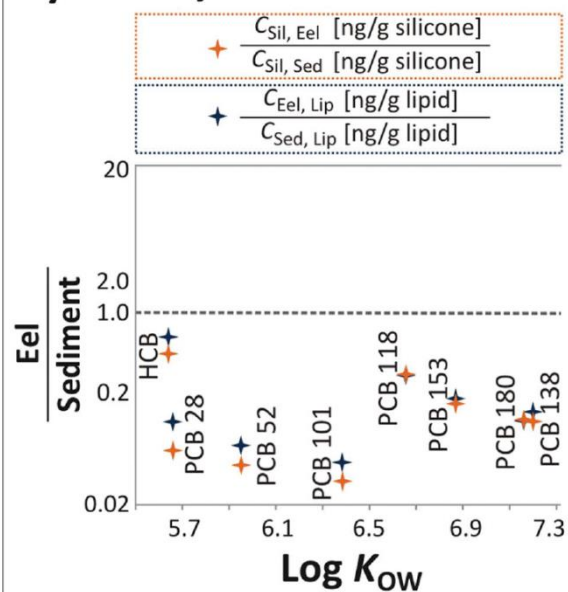
Cite this: *Environ. Sci.: Processes Impacts*, 2014, 16, 464



A) BSAFs

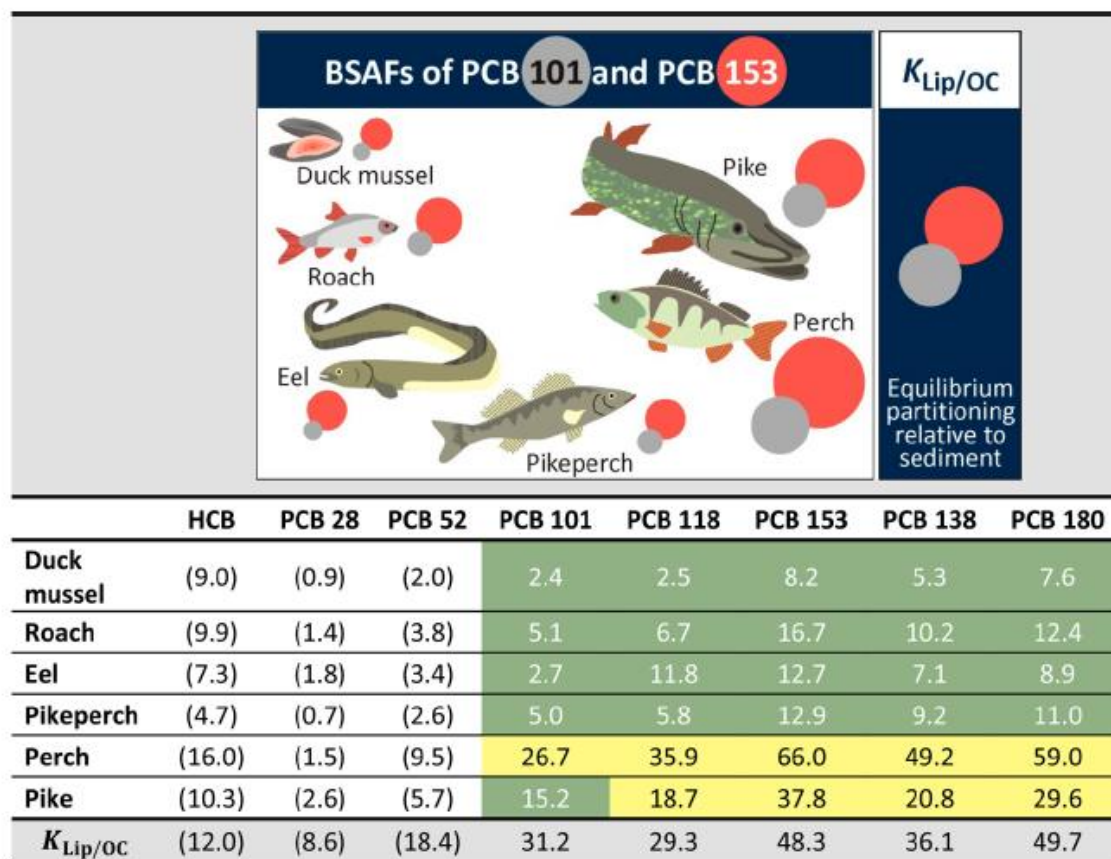


B) Activity ratios



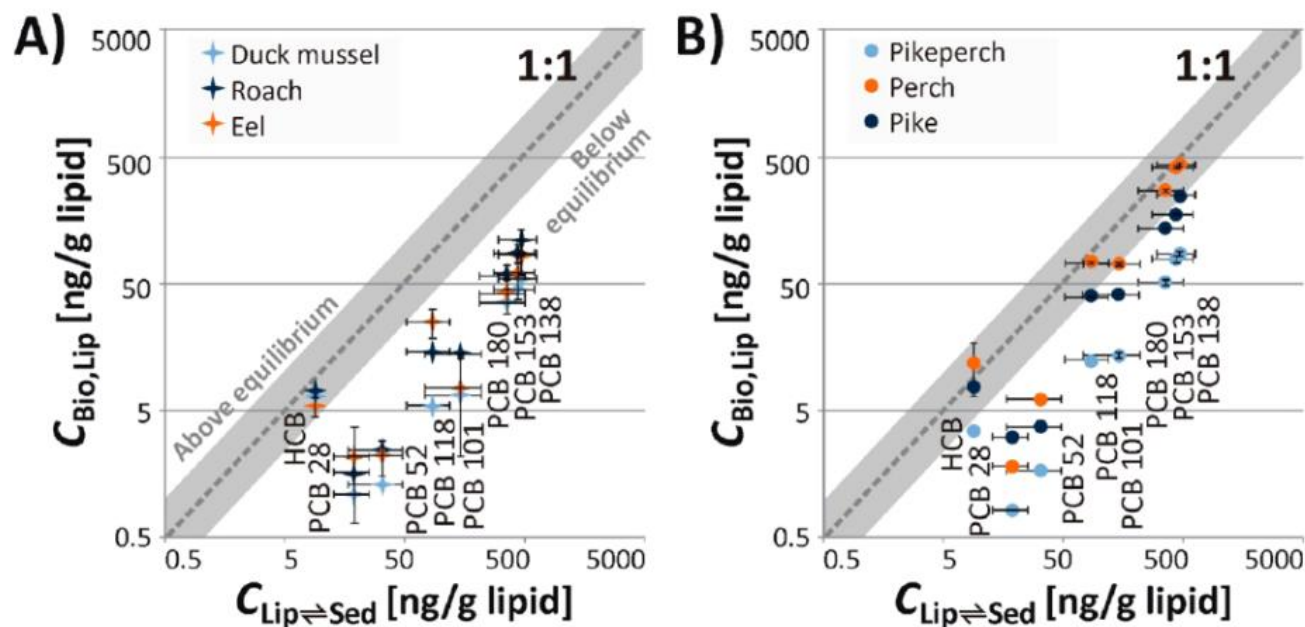
Equilibrium Sampling to Determine the Thermodynamic Potential for Bioaccumulation of Persistent Organic Pollutants from Sediment

Annika Jahnke,^{*,†} Matthew MacLeod,[†] Håkan Wickström,[‡] and Philipp Mayer[§]



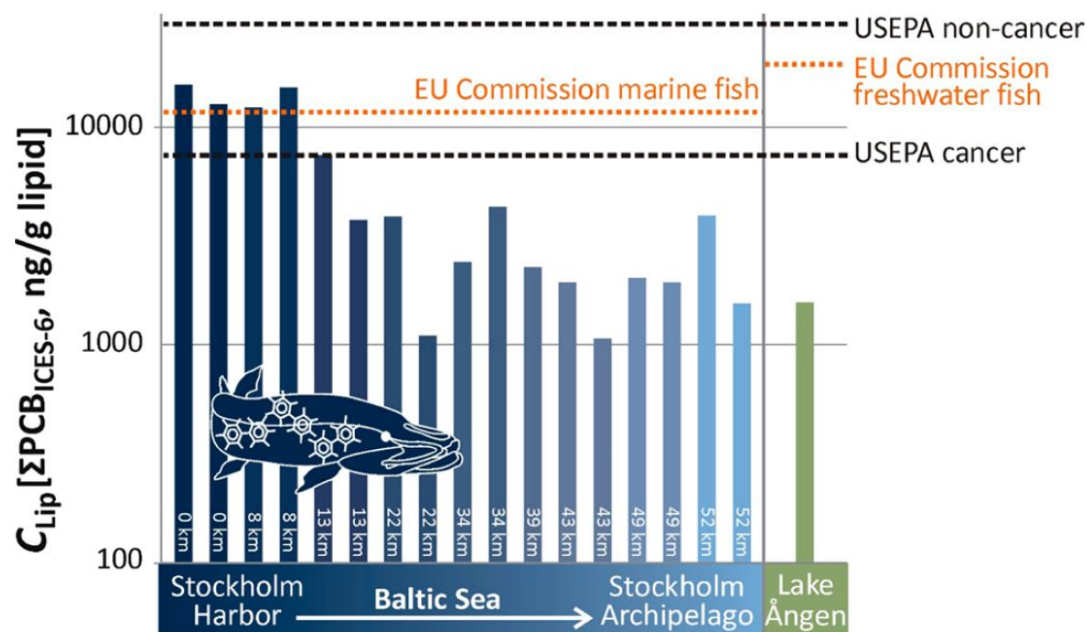
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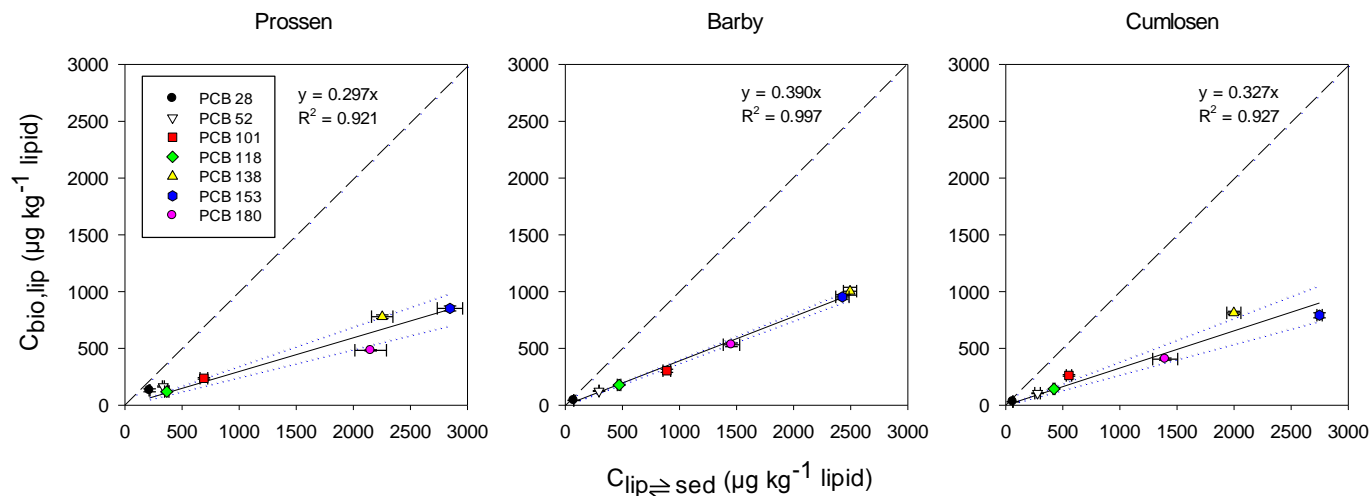


Equilibrium sampling of polychlorinated biphenyls in River Elbe sediments – Linking bioaccumulation in fish to sediment contamination



Sabine Schäfer^{a,*}, Catherine Antoni^{a,1}, Christel Möhlenkamp^a, Evelyn Claus^a, Georg Reifferscheid^a, Peter Heininger^a, Philipp Mayer^b

1. ex situ equilibrium sampling of sediment from 10 locations in River Elbe (Germany)
2. $C_{\text{lipid-normalized}}$ in common bream from independent monitoring program



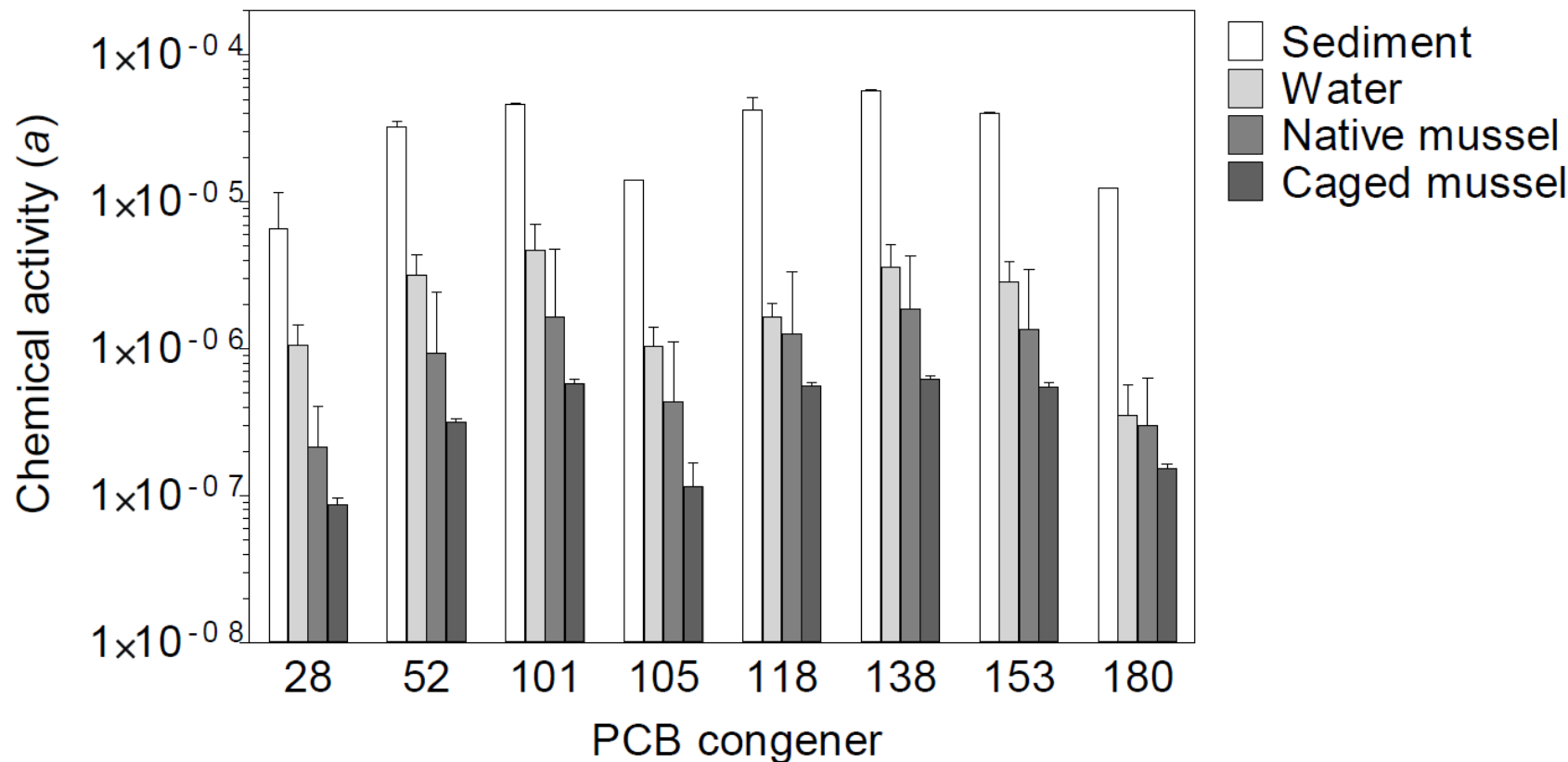
1. Cross validation of two monitoring programs
2. Bioaccumulation in common bream tightly linked to $C_{\text{lip=sed}}$
 - $R^2 > 0.9$ (linear scale!) & very similar slopes between sites

5)

ET&C, 2015, V 34: 2463–2474 (DOI: 10.1002/etc.3099)

Fate of polychlorinated biphenyls in a contaminated lake ecosystem: Combining equilibrium passive sampling of sediment and water with total concentration measurements of biota

Kimmo Mäenpää, Matti Leppänen, Kaisa Figueiredo, Philipp Mayer, Dorothea Gilbert, Sirpa Herve, Annika Jahnke, Carmen Gil-Allué, Jarkko Akkanen, Inna Nybom, Auli Kostamo



Quantitative Thermodynamic Exposure Assessment (Q-TEA) Supporting Resilient Contaminated Sediment Site Restoration

USACE-ERDC (Lead): Todd S. Bridges, Philip T. Gidley, Guilherme Lotufo, Carlos Ruiz, Alan J. Kennedy,

DTU: Philipp Mayer, Stine Nørgaard Schmidt

Sediment Solutions: Upal Ghosh

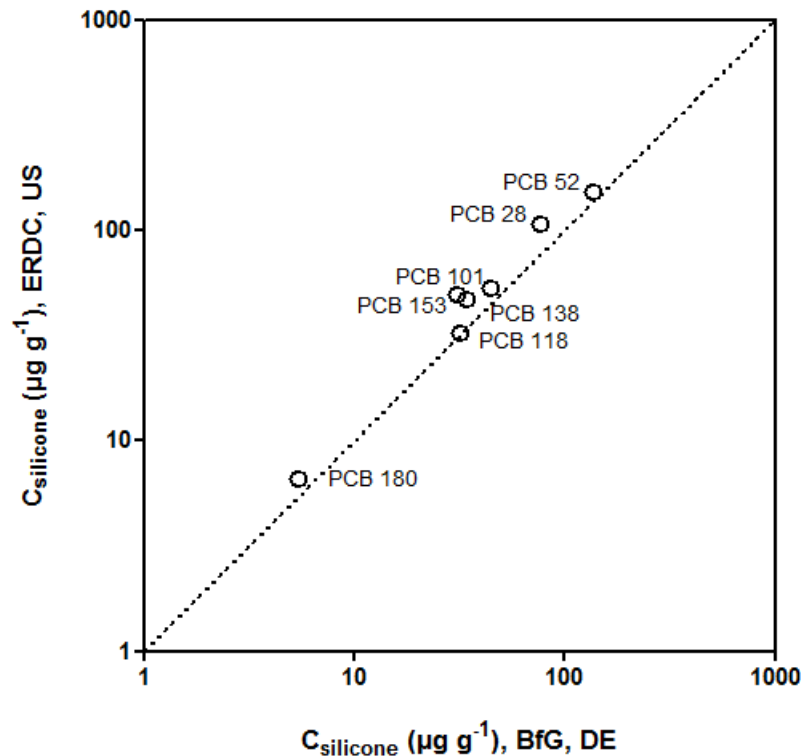
USA-EPA: Robert M. Burgess

Northeastern University: Loretta Fernandez,



Cross validation of equilibrium sampling

1. Coated jars produced at DTU & BfG
2. Equilibrium sampling of New Bedford sediment at BfG & ERDC
3. Instrumental analysis at BfG & ERDC



Conclusions and take home messages

Equilibrium sampling of sediments

- equilibrium sampling feasible even for PCBs
- can yield C_{free} , chemical activity & $C_{\text{lip} \rightleftharpoons \text{sed}}$

$C_{\text{lip} \rightleftharpoons \text{sed}}$

- in all studies so far $\geq C_{\text{lipid,normalized}}$
- thermodynamic potential for bioaccumulation

Sediments have high PCB levels, not only in concentration but also thermodynamically!

Acknowledgements

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